Mississippi State University: Center for Advanced Vehicular Systems

Tribology and Friction of Soft Materials: Mississippi State Case Study

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Advanced Materials: Models and Methods Forum
March 18, 2010

## Report Documentation Page

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1. REPORT DATE **18 MAR 2010**	2. REPORT TYPE **N/A**	3. DATES COVERED **-**	
4. TITLE AND SUBTITLE **Tribology and Friction of Soft Materials:Mississippi State Case Study**		5a. CONTRACT NUMBER **W56 HZV-08-C-0236**	
		5b. GRANT NUMBER	
		5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) **J.L. Bouvard; E.B. Marin; D. Oglesby; K. Solanki; B. Kirkland; M.F. Horstemeyer; P. Wang; R.L. King**		5d. PROJECT NUMBER	
		5e. TASK NUMBER	
		5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Mississippi State University:Center for Advanced Vehicular Systems**		8. PERFORMING ORGANIZATION REPORT NUMBER **20625**	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) **US Army RDECOM-TARDEC 6501 E 11 Mile Rd Warren, MI 48397-5000, USA**		10. SPONSOR/MONITOR'S ACRONYM(S) **TACOM/TARDEC**	
		11. SPONSOR/MONITOR'S REPORT NUMBER(S) **20605**	
12. DISTRIBUTION/AVAILABILITY STATEMENT **Approved for public release, distribution unlimited**			
13. SUPPLEMENTARY NOTES **The original document contains color images.**			
14. ABSTRACT			
15. SUBJECT TERMS			

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT **SAR**	18. NUMBER OF PAGES **24**	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**			

Outline

1. Background of Mississippi State U.

2. MSU/CAVS Capabilities

3. Overall Strategy for Polymer Research

4. Multiscale Material Modeling

5. Case Study

6. Summary

Mississippi State University:
Center for Advanced Vehicular Systems
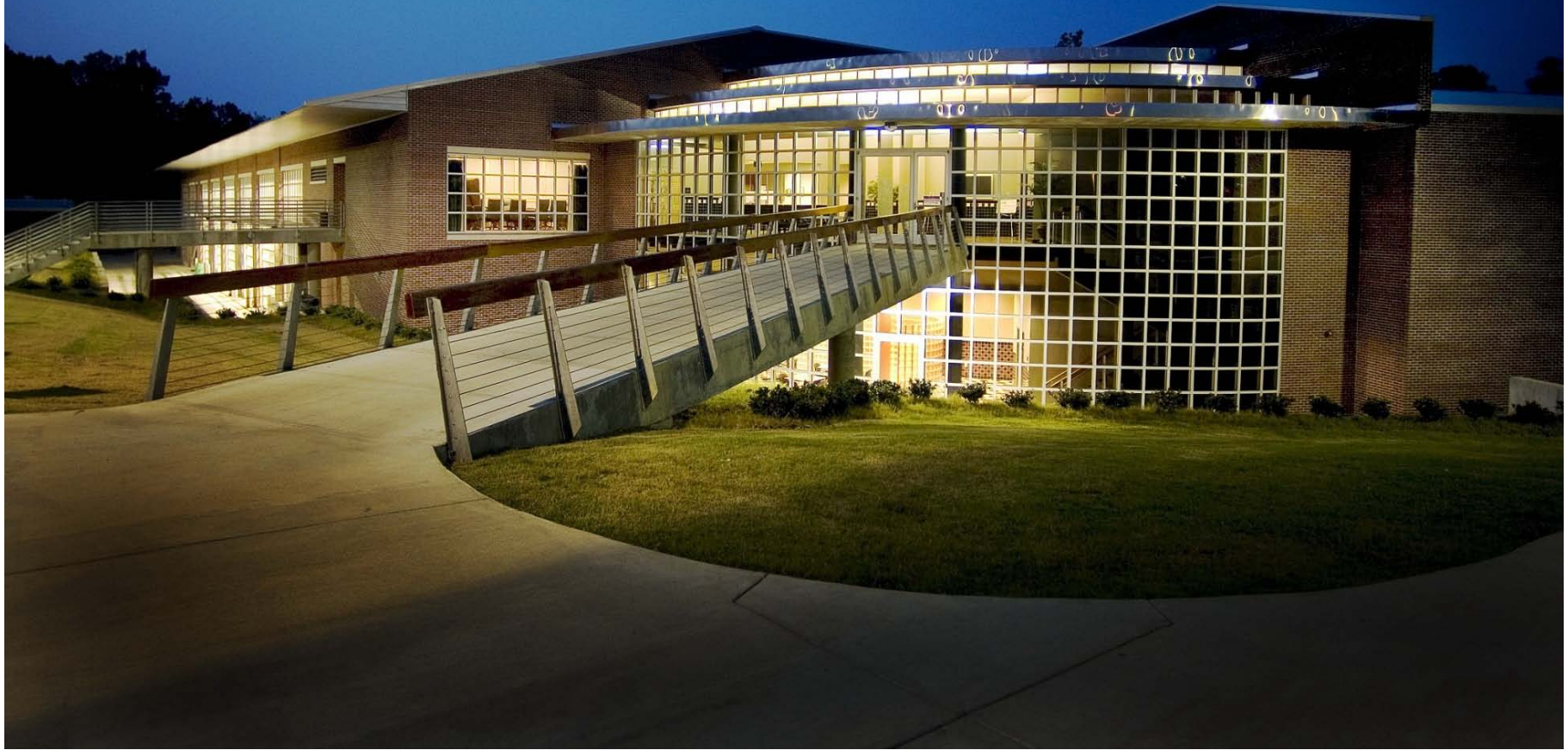
www.cavs.msstate.edu

Bagley College of Engineering Degree Programs

Mechanical Engineering

Industrial Engineering

Software Engineering (Undergraduate only)

Applied Physics (Graduate only)

Aerospace Engineering

Electrical Engineering

Biological Engineering

Computer Science

Biomedical Engineering (Graduate only)

Computational Engineering (Graduate only)

Chemical Engineering

Civil Engineering

Computer Engineering

CAVS Today

CAVS STRENGTH: People (about 250)

Faculty: 47

Staff: 58

Graduate students: 85

Undergraduate students: 79

CAVS GOAL: Become the nation's premier interdisciplinary high-performance *vehicular* computing research facility.

NEXT STEPS: CAVS has a central focus on computational engineering to serve as our differentiator. We have now broadened the domain definition of the term "vehicular." We are in the process of defining areas of research which are needed to complement the central focus.
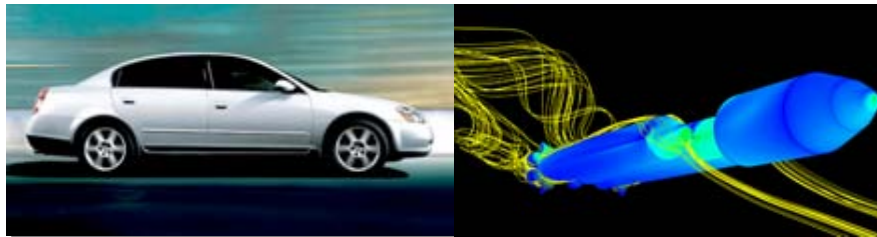
CAVS/MSU Capabilities

➢ **Materials Characterization Facilities**
X-Ray CT Scan, High performance FEG-SEM, EVO–SEM, TALYSURF CLI 2000, Hysitron Nanoindenter, Axiovert Optical Microscope, Particle Size Analyzer, Spectroscopy, …

➢ **High Temperature Characterization Facilities**
TGA, DSC, DMA, Dilatometer, Microwave Sintering Furnace, Arburg Powder Injection Molding, Randcastle–Extruder, Powder Compaction Machine, …

➢ **Mechanical Properties - Testing Facilities**
Hopkinson Bar setup (compression, tension, and torsion), Instron (50 kN, and 100 kN load capacity), Biaxial Instron, MTS (5-25 kN load capacity), Hardness Tester, Structural Test Systems, …

➢ **Computational capabilities**

SunFire X2200 M2 (2048 Opteron proc.), IBM x335 Linux Supercluster (384 Pentium IV proc.), IBM x300 Linux Supercluster (1038 Pentium proc.), UltraSparc SUN

Websites:
http://www.cavs.msstate.edu/cavs4capabilities.php
http://www.dial.msstate.edu/cap/Analytical%20Services%20Laboratory%20Web%20Page%20August%202006.html
http://emcenter.msstate.edu

Polymer Overall Strategy (1)

Motivation

1. Increase the reliability and safety involving designing with polymeric materials for the automotive industry.
2. Better understanding of the mechanical response of polymers
3. Building a material database and developing material models for these materials

Modeling the Mechanical Response of Polymers

Experiments — DMTA, TMS, SHPB

Structure-Property Relationships — transitions, strain-stress curves

Modeling — mechanical model, constitutive equations

Goals

A. Develop material database capturing structure-property relationships for thermoplastics, elastomers, foams, and fabrics.

B. Develop internal state variable (ISV) material model. Model will be calibrated using database and verified / validated for a range of strain rates and temperatures.

Materials

Plastics:

Polycarbonate (PC)
Acrylonitrile Butadiene Styrene (ABS)
Polypropylene (PP)

Rubbers

Natural rubber
Santoprene (Vulcanized Elastomer)
Styrene Butadiene Rubber (SBR)

Foams

Polypropylene Foam
Polyurethane Foam

Fabrics

Kevlar
Nylon

Polymer Overall Strategy (2)

Experiments

Mechanical Tests

- Low to High strain rates

- Temperatures below/above Tg

- Volumetric testing, relaxation,
  dissipation, strain paths,
  stress state)

- Impact tests

- Fatigue tests

Mechanical / Fatigue tests
- Test at different strain rates, temperature, Hz
(stress/strain ratios, cyclic loading to failure)
Micro-structural studies
- Failure mechanisms (crack initiation / growth)

Materials

PLASTICS
Polycarbonate (PC)
Polypropylene (PP)
ABS

RUBBERS
Natural Rubber
Santoprene
SBR
TPU

FOAMS
PP foam
PU foam

Modeling / Simulation

ISV material model (improved):
- Identification / Calibration
- FEA Implementation (ABAQUS,)
- Verification

Fatigue model:
- Identification / Calibration
- FEA Implementation (ABAQUS,)
- Verification

ISV material model:
- Identification / Calibration
- FEA Implementation (ABAQUS,)
- Verification

Fatigue model:
- Identification / Calibration
- FEA Implementation (ABAQUS)
- Verification

Work supported by:
TARDEC (DoD)
American Chemistry Council
DOE

People: **Faculty (8), Staff (3), PhD (3), UG (10)**

Multiscale Polymer Modeling

Bridge 12 = FEA

ISV

Bridge 11 = FEA

Macroscale ISV Continuum

Nanoparticle/ crack Interactions

Bridge 10 = Nanoparticle, polymer interactions

Fracture mechanics (ISV + FEA)

100-500µm

Bridge 5 = Particle-Void Interactions

Bridge 9 = Bonding, mobility

Micromechanics (ISV and FEA)

10-100 µm

Bridge 8 = Density, T effects

Bridge 4 = Particle Interactions

Bridge 7 = High Rate Mechanisms

Coarse graining MD and MC

Bridge 3 = Hardening Rules

100's Nm

Coarse graining

Bridge 6 = Elastic Moduli

Bridge 2 = Mobility

Nm

Atomistics (EAM,MEAM,MD,MS)

Bridge 1 = Interfacial Energy, Elasticity

Å

Electronics Principles (DFT)

Studying Polymers with Molecular Dynamics

Typical terms in Inter-atomic potential

Bond angle

$$E_{bs}(r) = \sum_{atoms} \{k_r(r - r_0)^2\} \quad \longleftarrow \quad \text{Bond stretching}$$

$$E_{be}(,) = \sum_{atoms} \{k_{,}(,-,_0)^2\}$$

$$E_{to}(\square) = \sum_{atoms} \{V_1\cos\square + V_2\cos 2\square + V_3\cos 3\square + V_6\cos 6\square\}$$

$$E_{vw}(\bar{r}) = \sum_{nobonded} \{A(\bar{r})^{-12} - C(\bar{r})^{-6}\}$$

Bond torsion

Van der Waals
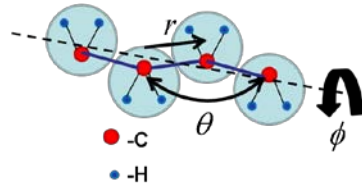
Nanoscopic specimen of idealized Linear amorphous polyethylene under uniaxial tension (T=100K, nc=200, n_monomers=1000)

Van der Waals interaction

Chains alignment (bond torsion)
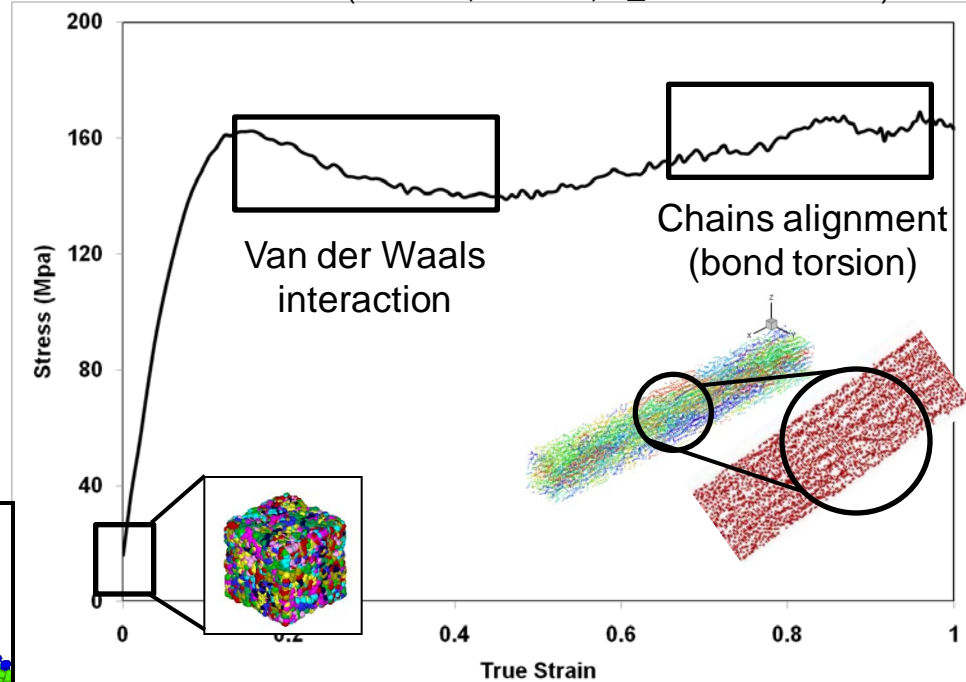
Multiscale Polymer Modeling
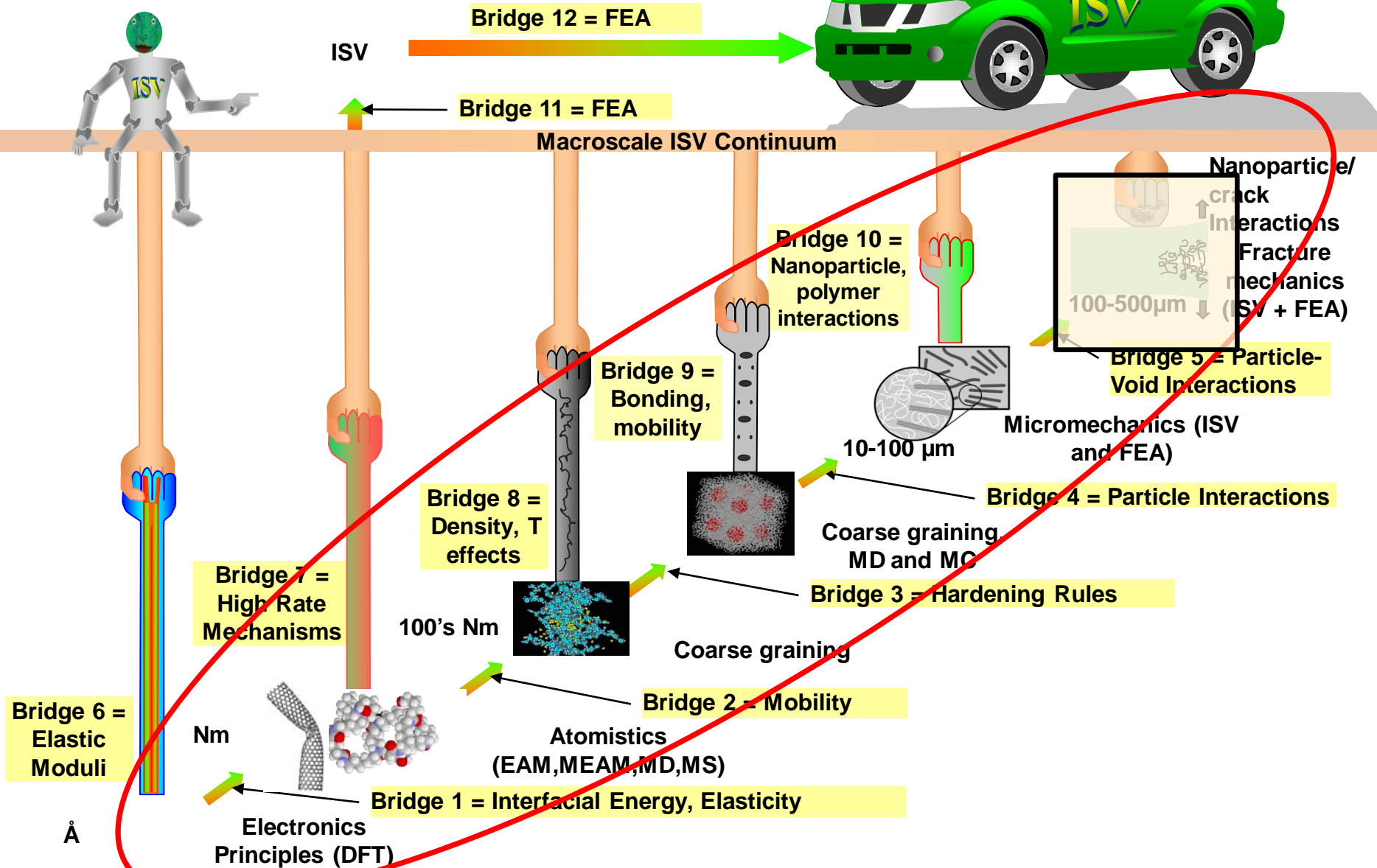
Methodology Applied to Model Mechanical Response of Polymers

Polycarbonate
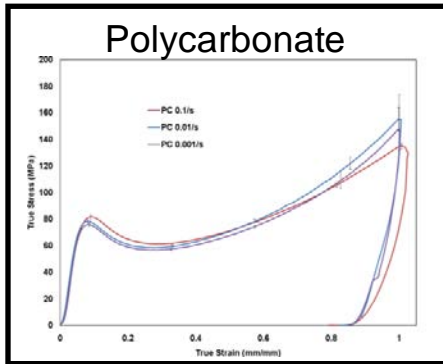
EXPERIMENTAL DATA

ISV MATERIAL MODEL

3-D Constitutive Equations + Numerical Integration Procedure

fitting algorithm developed for MATLAB

PC

1-D Constitutive Equations

MODEL CALIBRATION TOOL
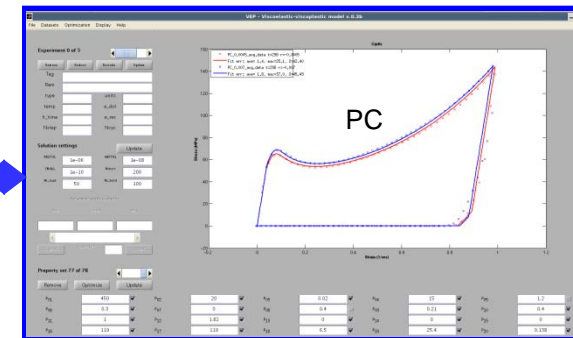
Impact Problem (ABAQUS Explicit)

striker

Axisymmetric rigid elements RAX2

Axisymmetric deformable elements CAX4R
Size 0.1 mm and 1.45 mm

PC Disk

Adaptive mesh domain

Axially symmetric model
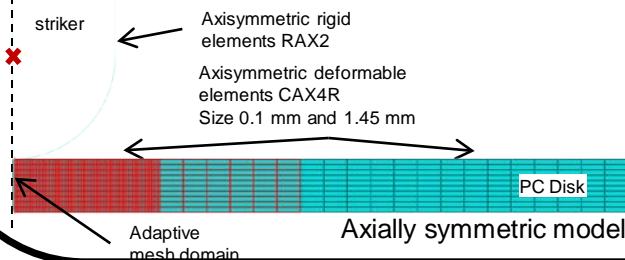
FEA

Numerical Implementation in FEM Codes

Multiscale Experiments

16,000x

3.5mm Extension | 11.5mm Extension | 15.0mm Extension

Void Nucleation

Void Coalescence

Void Coalescence — 16.3mm Extension
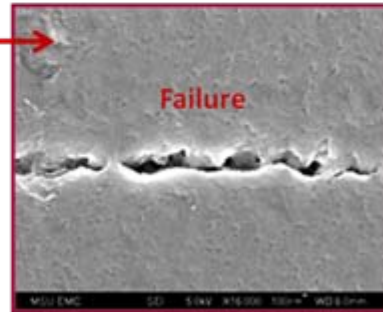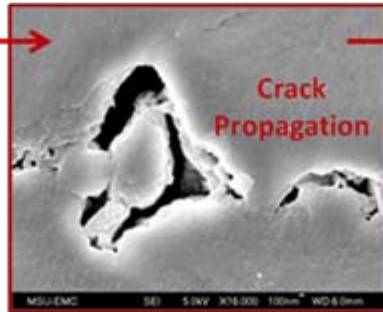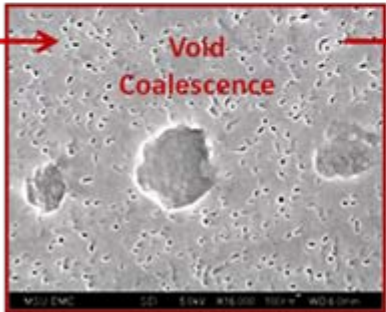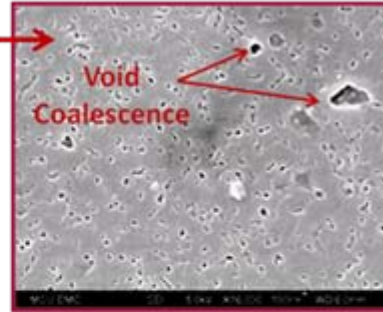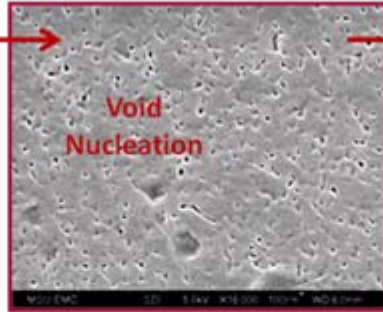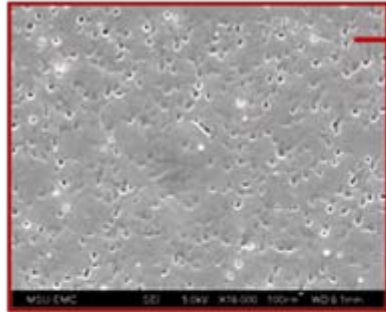
Crack Propagation — 49.0mm Extension

Failure — Extension Until Failure

Nanoscale

Model — Cohesive Energy Critical Stress

Analysis — Fracture Interface Debonding

Experiment — TEM

Microscale

Experiment — SEM Optical methods

ISV Model — Void Nucleation

FEM Analysis — Idealized Geometry Realistic Geometry

Mesoscale

Experiment — Fracture of Silicon Growth of Holes

ISV Model — Void Growth Void/Crack Nucleation

Fem Analysis — Idealized Geometry Realistic RVE Geometry Monotonic/Cyclic Loads Crystal Plasticity

Multiscale Experiments

1. Exploratory exps
2. Model correlation exps
3. Model validation exps

Structural Scale
Experiments → FEM

Nanoscale
Model — Cohesive Energy Critical Stress
Analysis — Fracture Interface Debonding
Experiment — TEM

Macroscale
Experiment — Uniaxial/torsion, Notch Tensile, Fatigue Crack Growth, Cyclic Plasticity
Continuum Model — Cyclic Plasticity Damage
FEM Analysis — Torsion/Comp, Tension, Monotonic/Cyclic

Microscale
Experiment — SEM, Optical methods
ISV Model — Void Nucleation
FEM Analysis — Idealized Geometry, Realistic Geometry

Mesoscale
Experiment — Fracture of Silicon, Growth of Holes
ISV Model — Void Growth, Void/Crack Nucleation
Fem Analysis — Idealized Geometry, Realistic RVE Geometry, Monotonic/Cyclic Loads, Crystal Plasticity

Compression Tests Results – Rubbers

Strain Rate Dependence (RT)
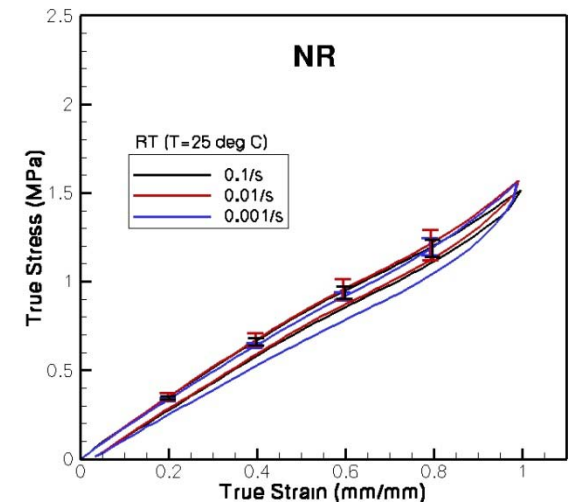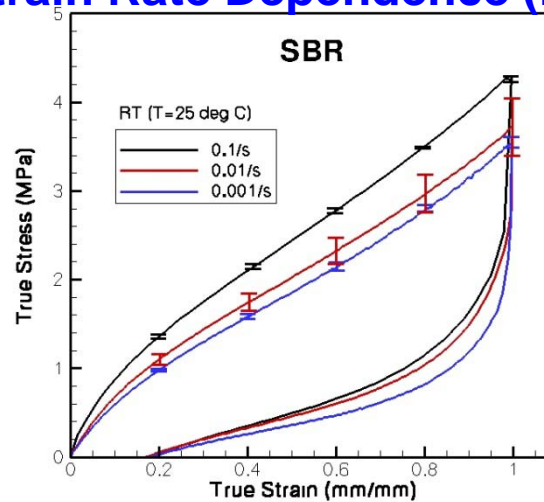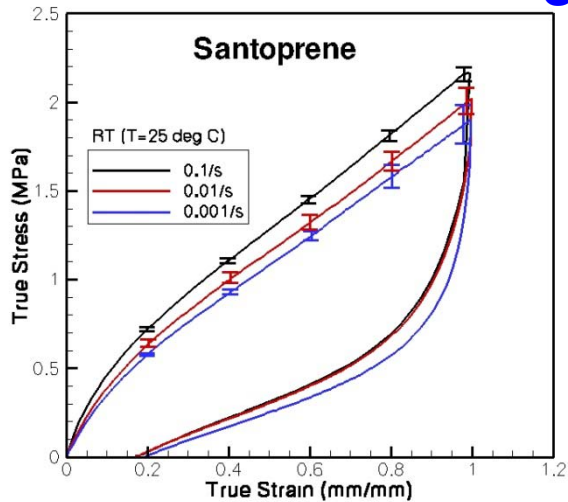
Temperature Dependence (0.01 /s)
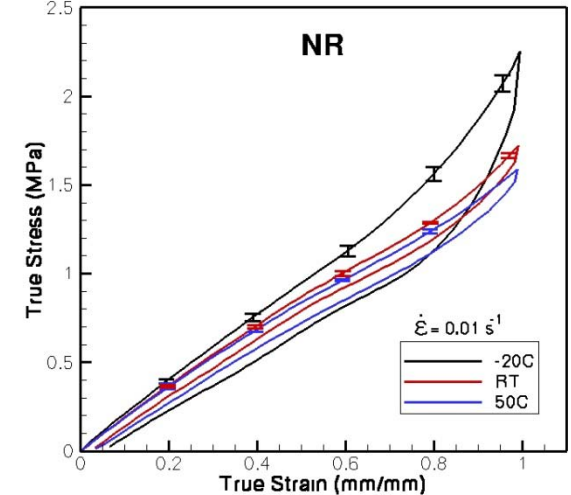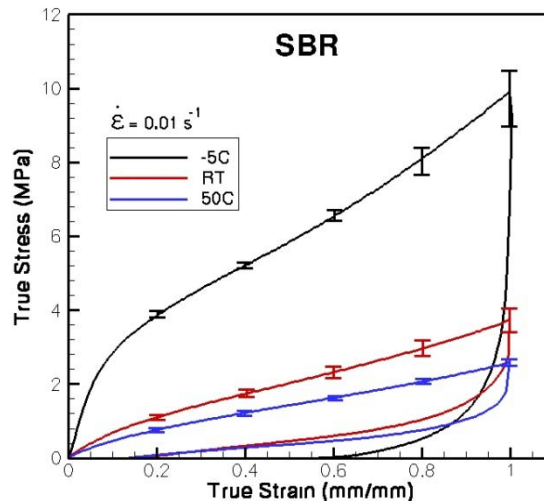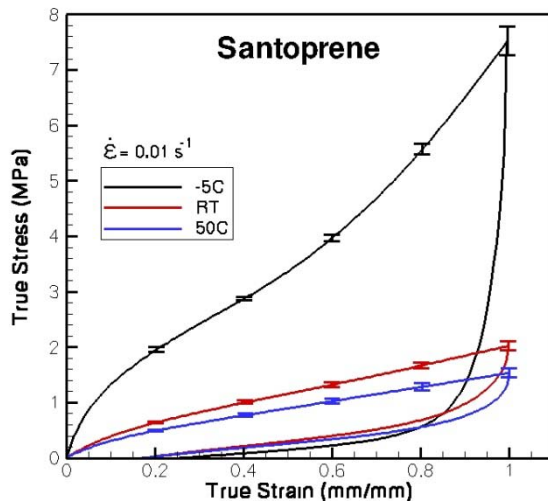
MSU/CAVS Case Study
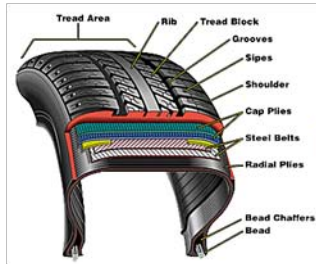
rubber tire

Michelin's PAX run-flat tire
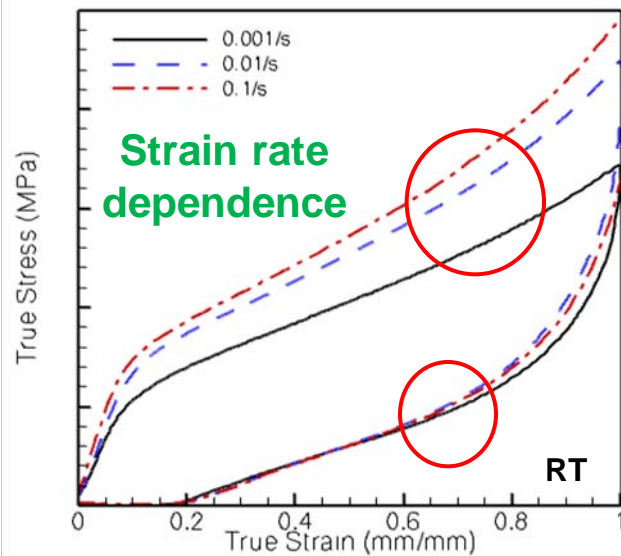

H.J. Qi and M.C. Boyce (2005)
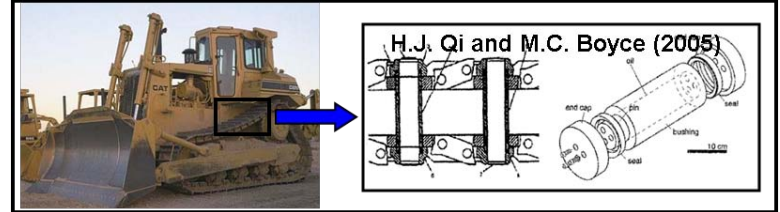
Goals

A. Capture experimentally the mechanical properties of Thermoplastic Polyurethane (TPU)

B. Develop an internal state variable (ISV) material model for this material.

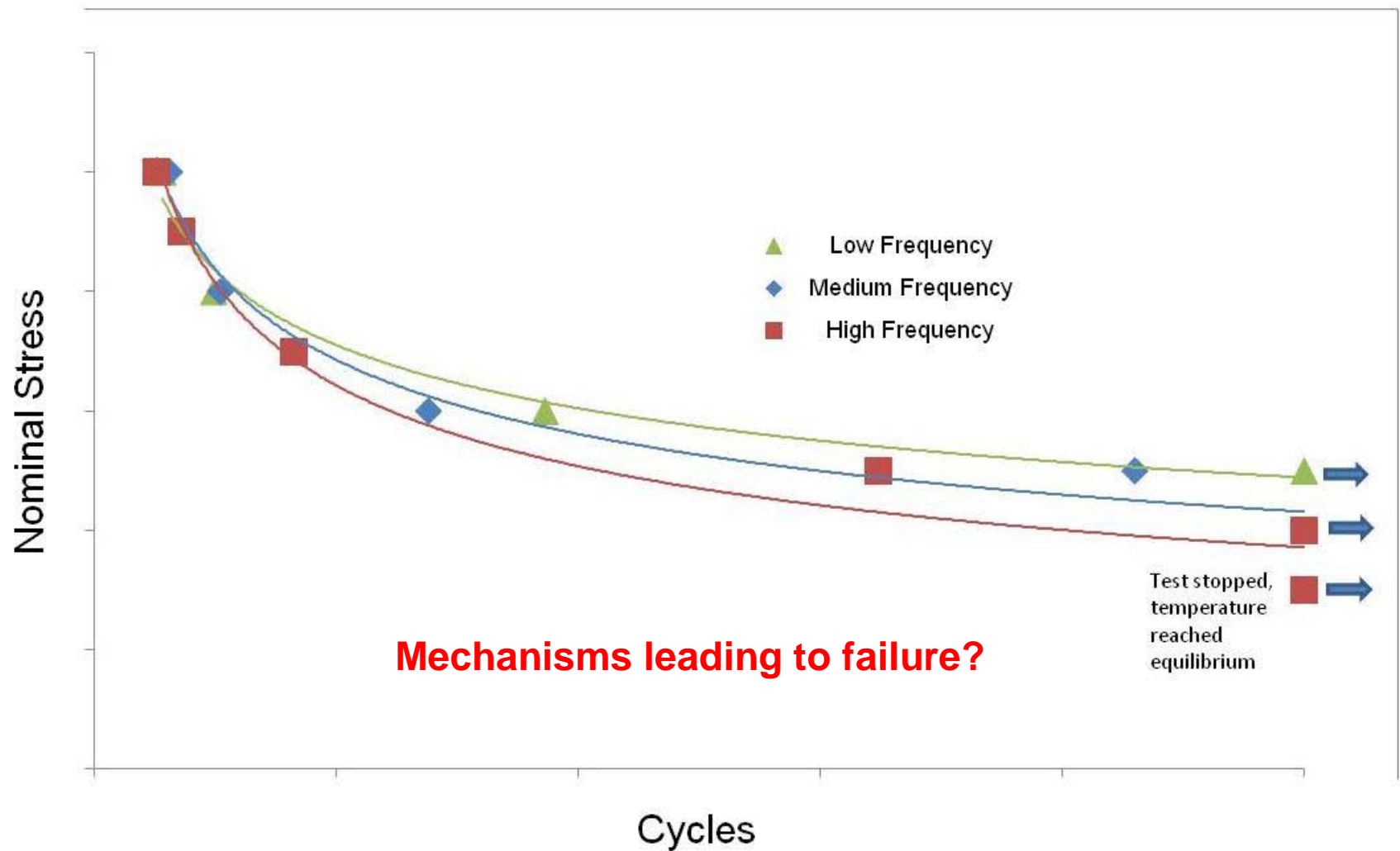**C**. Develop a preliminary multiscale fatigue model to predict the failure of real structural component

Approach

◆ Carry out experiments using current testing methodologies:
- Dynamic Mechanical Analyzer (DMA)
- Thermogravimetric Analysis (TGA)
- X-Ray Diffraction (XRD)
- INSTRON (tensile and compressive testing)

◆ Develop ISV material model
Develop a model calibration procedure (MATLAB)
Model implementation in finite element code (ABAQUS).

◆ Develop a Multiscale Fatigue Model

◆ Perform finite element analysis to understand/improve the the performance of a structural component design

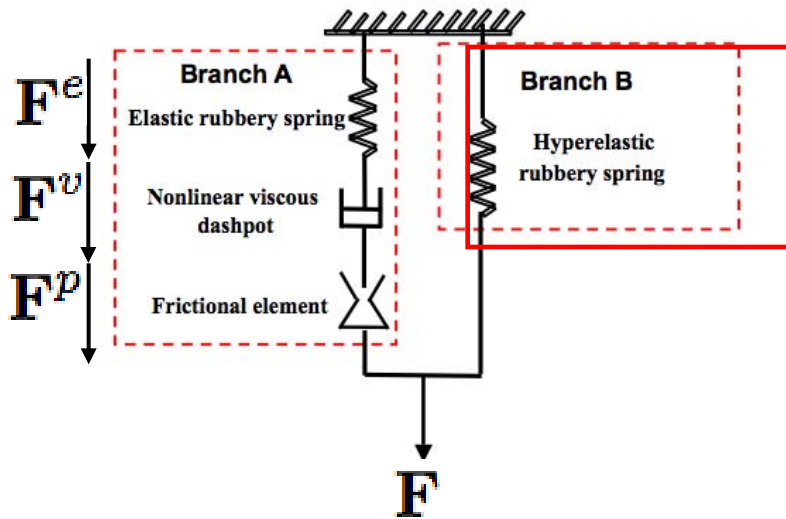# Mechanical Behavior at the Coupon Level (monotonic loading)
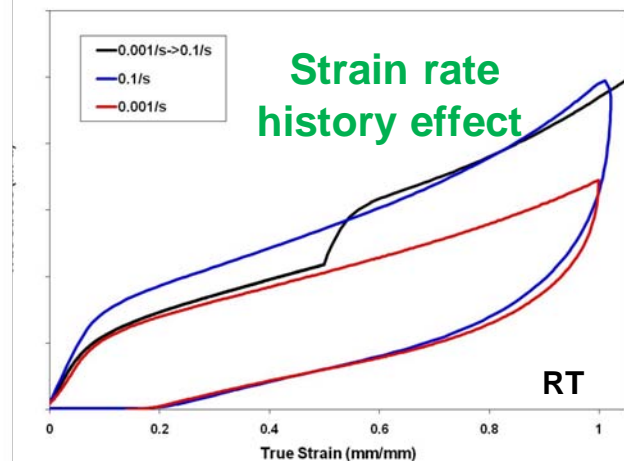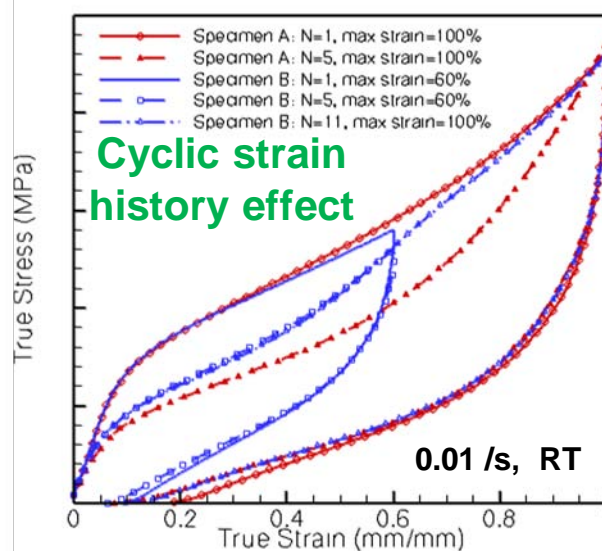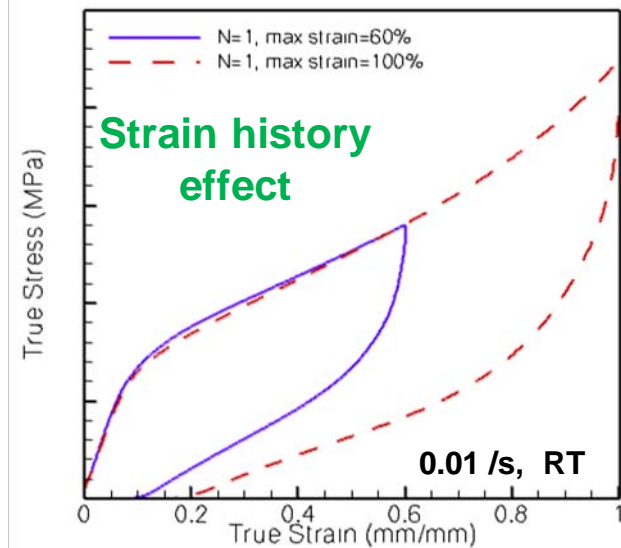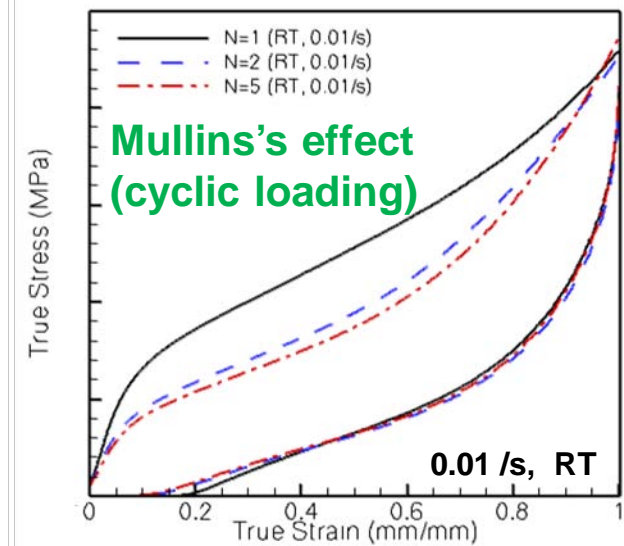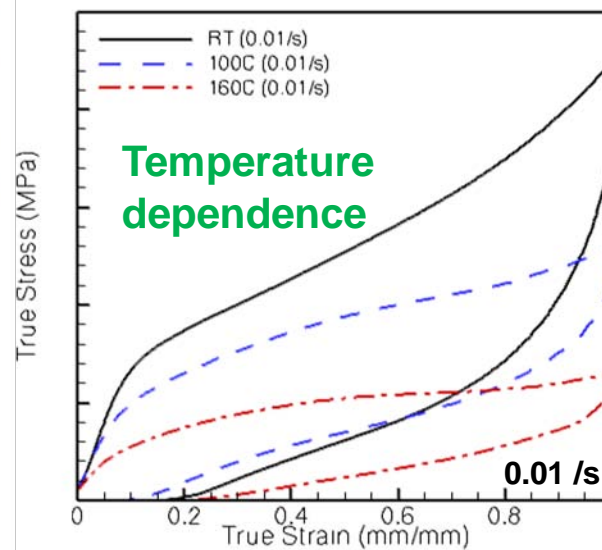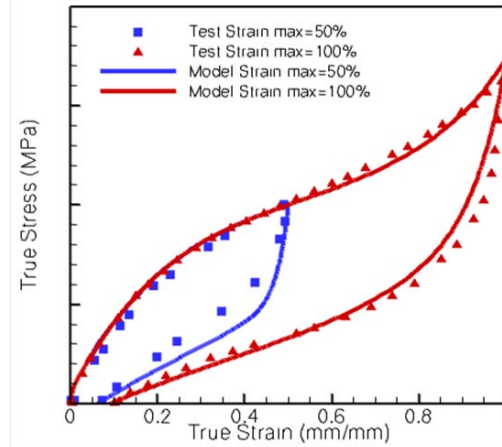
Stress – Life With Frequency Effects

Mechanisms leading to failure?

Fatigue Behavior: Internal Heat Build-up Leads to Failure

Failure = specimen deformed 5% from steady state length

Displacement

Temperature

Cycles

ISV Material Model Prediction

Branch A
- Elastic rubbery spring
- Nonlinear viscous dashpot
- Frictional element

Branch B
- Hyperelastic rubbery spring

$\mathbf{F}^e$
$\mathbf{F}^v$
$\mathbf{F}^p$
$\mathbf{F}$
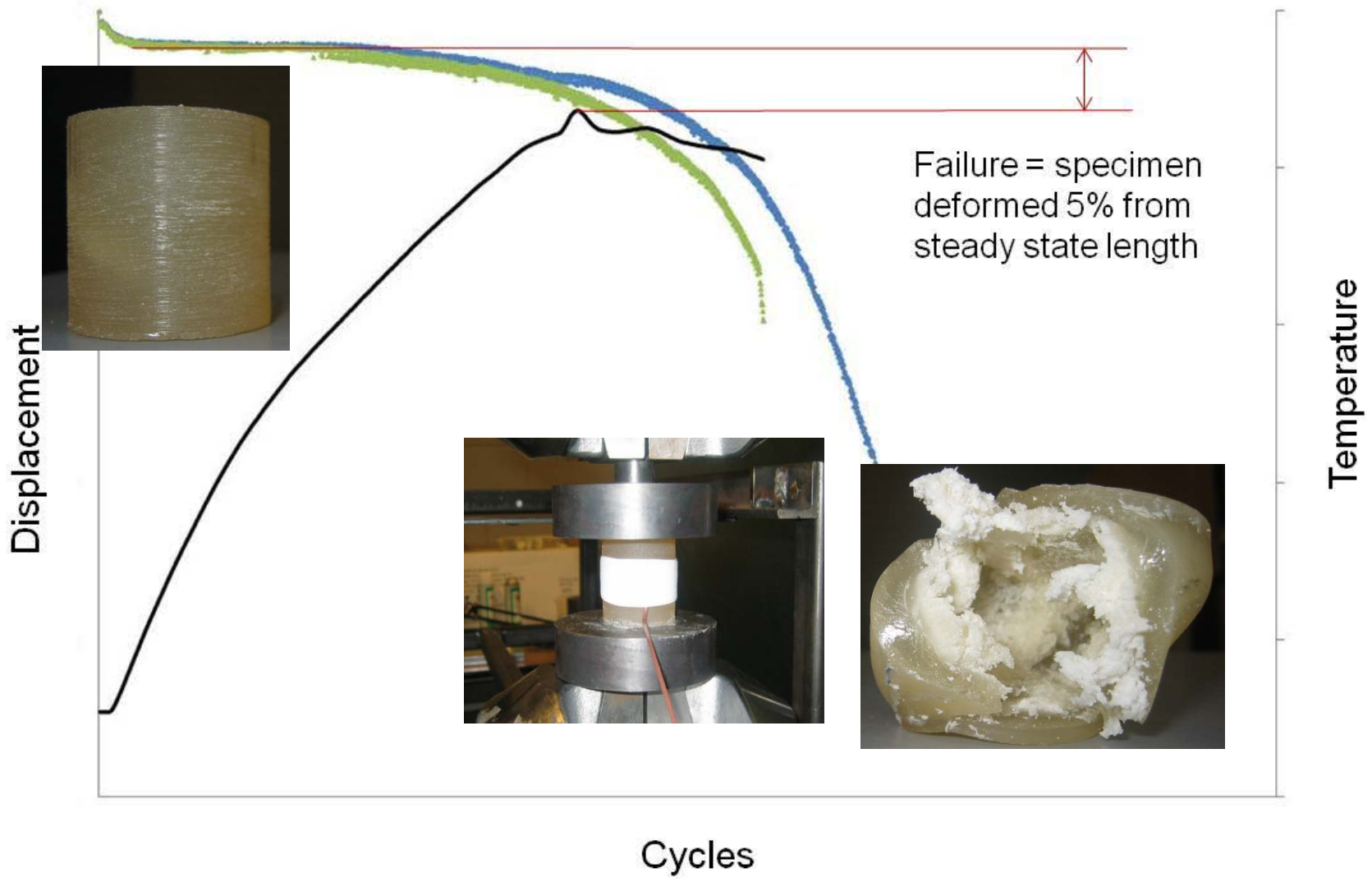
Maximum strain level
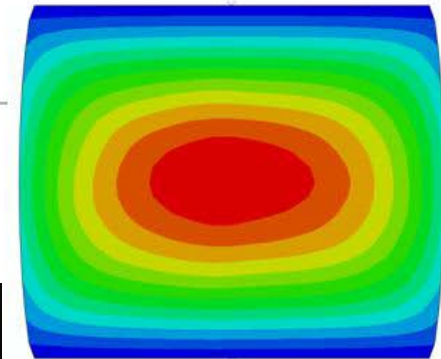

Mullins' effect
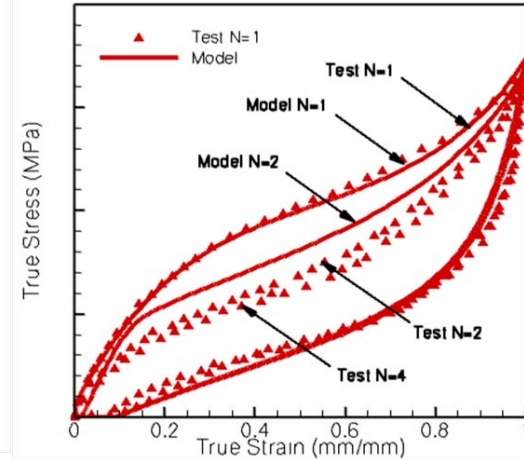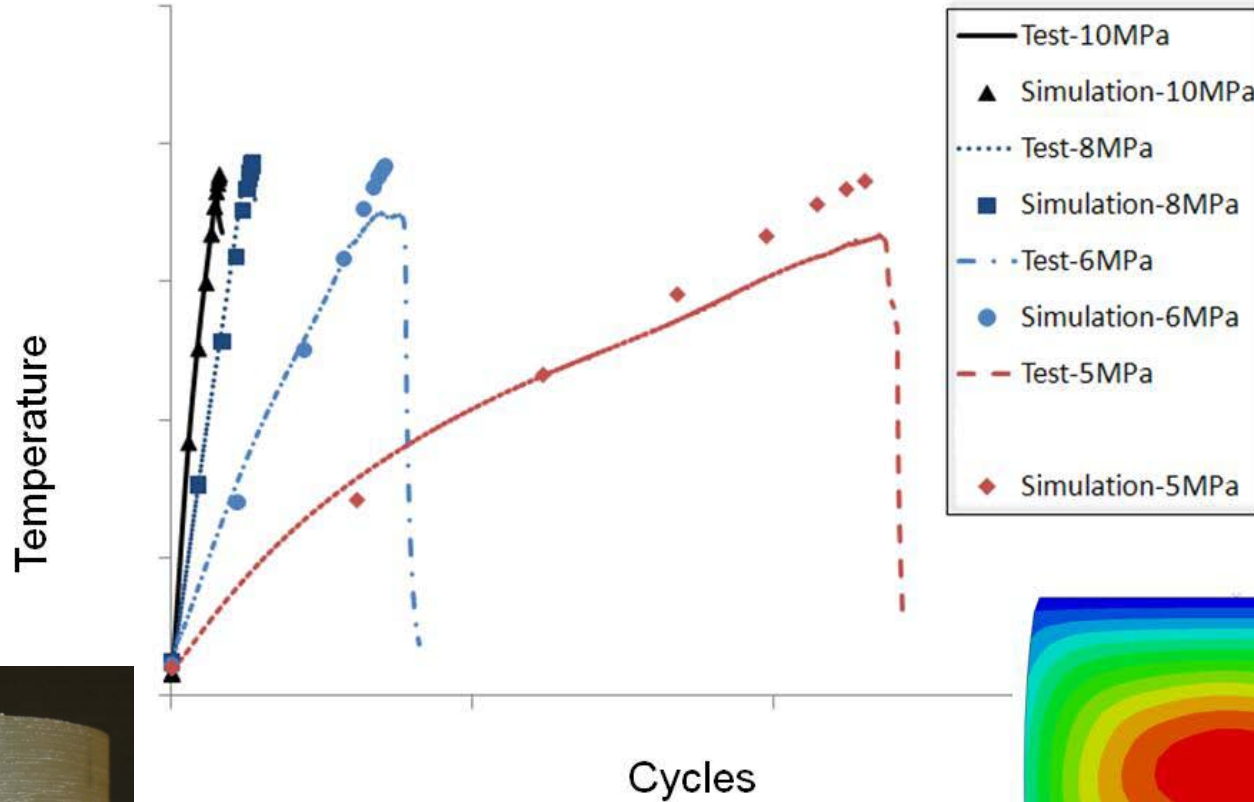

Relaxation tests
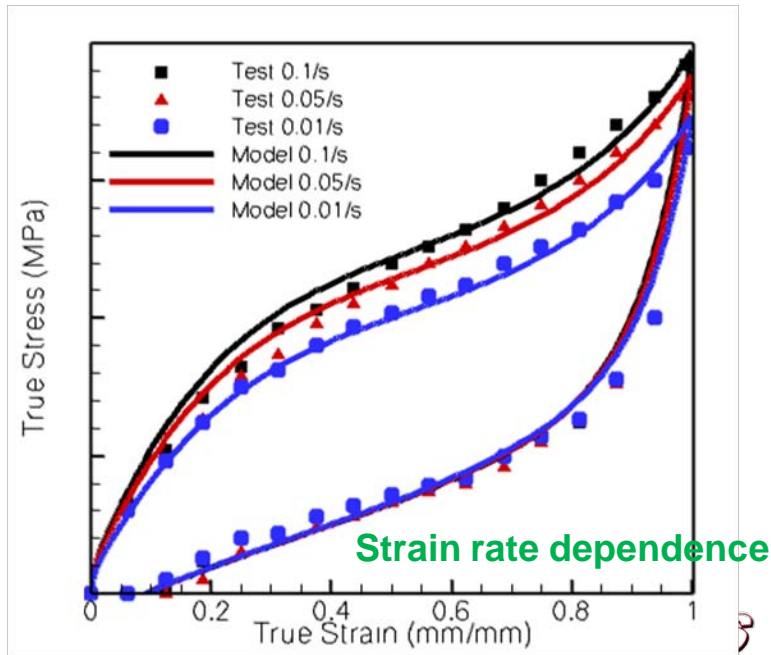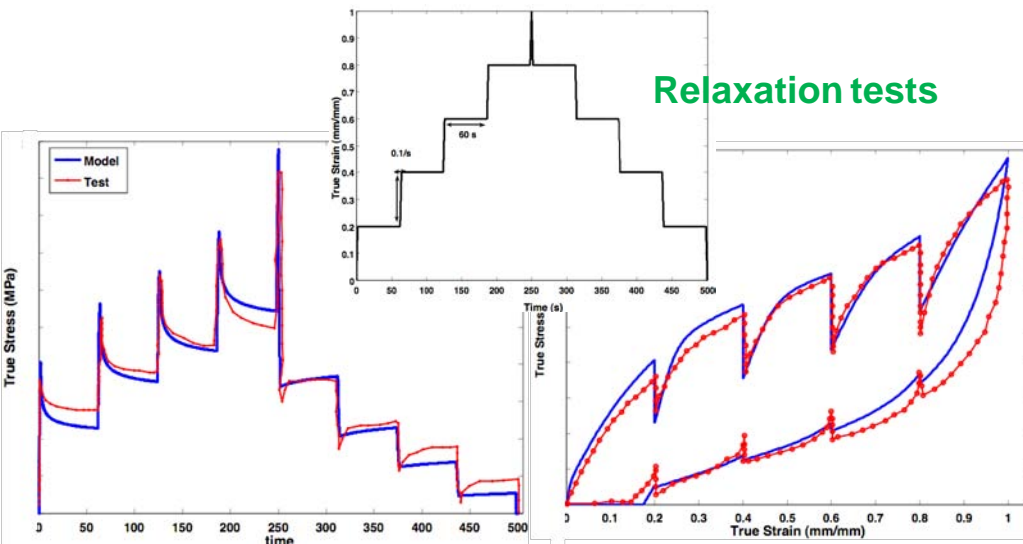
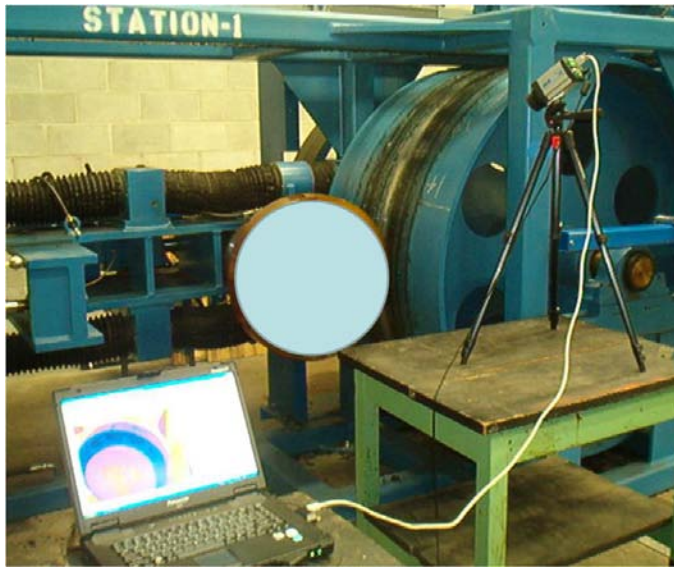

Strain rate dependence

ISV Material Model prediciton (isothermal problems)
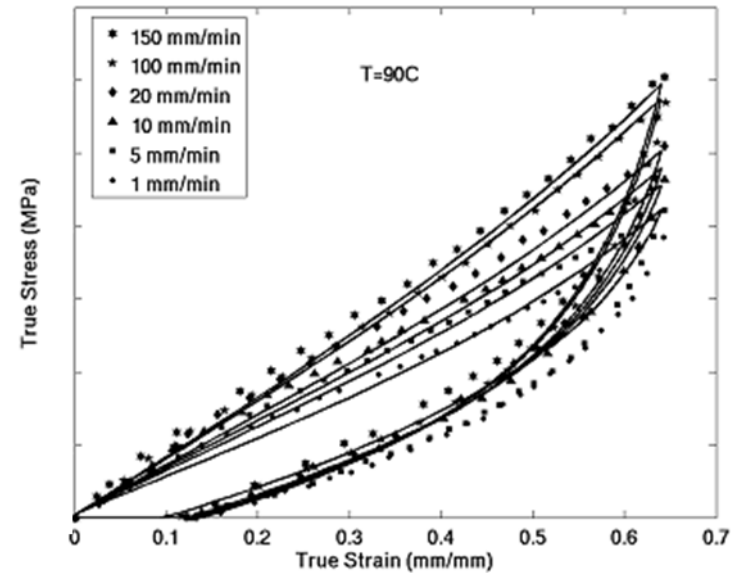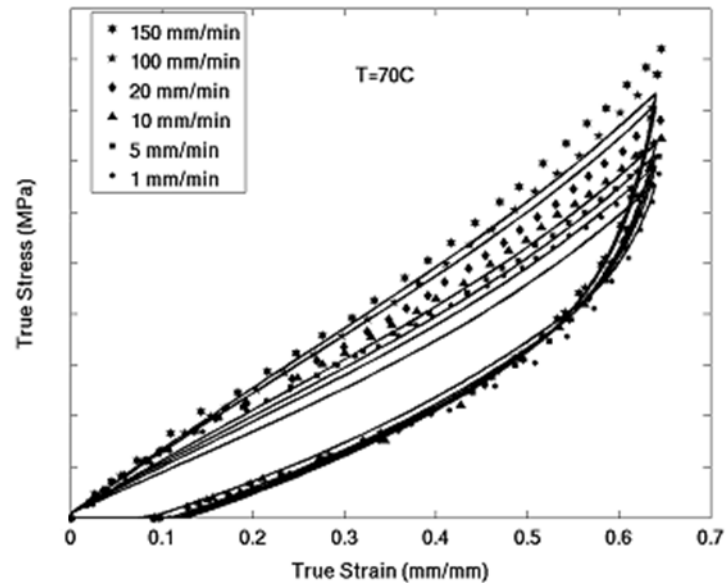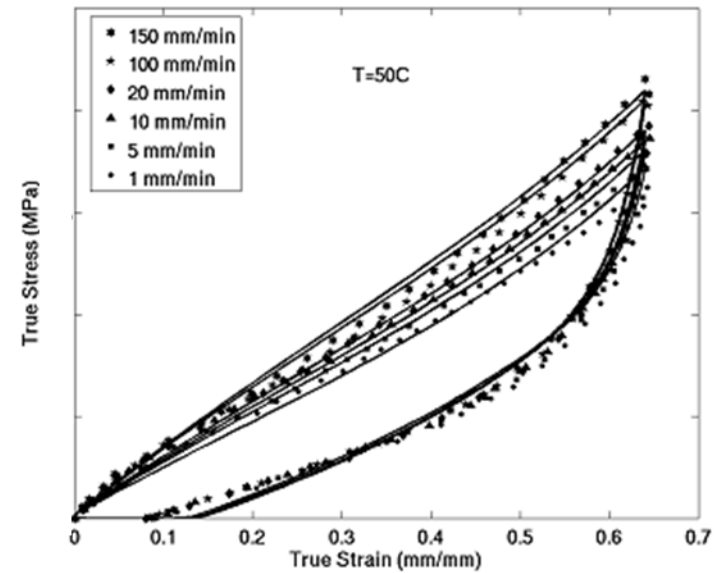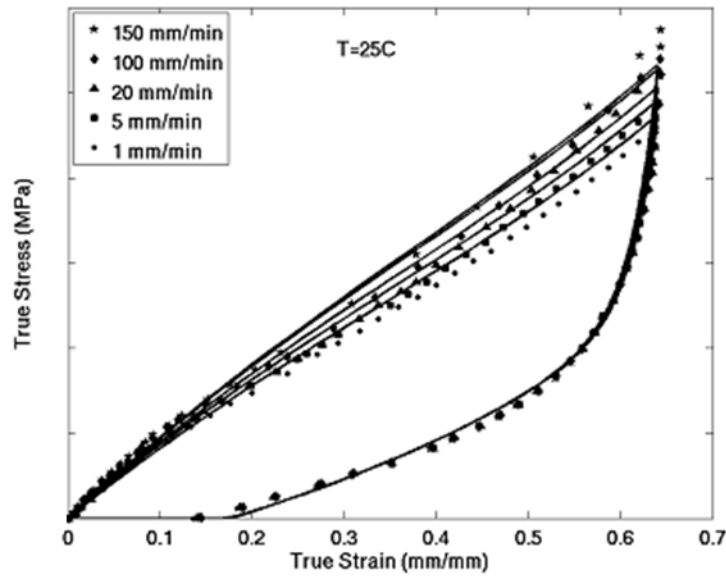
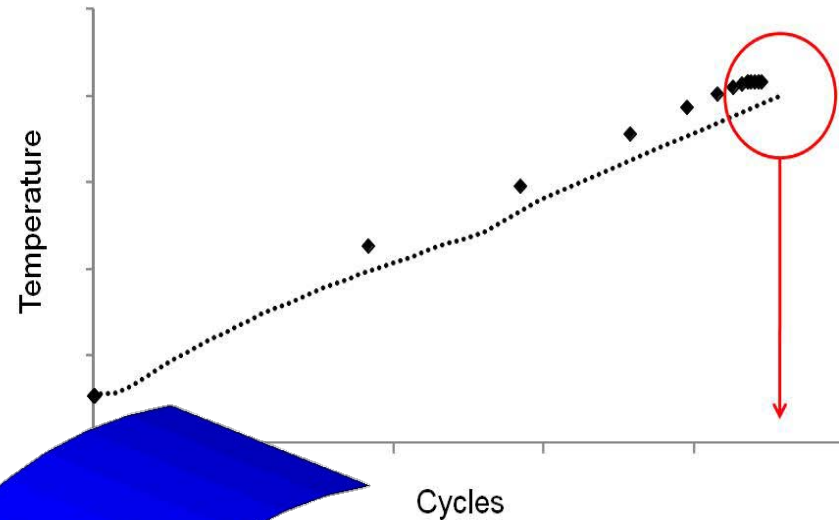# Thermal Fatigue Simulation at Medium Frequency for Various Stress Levels
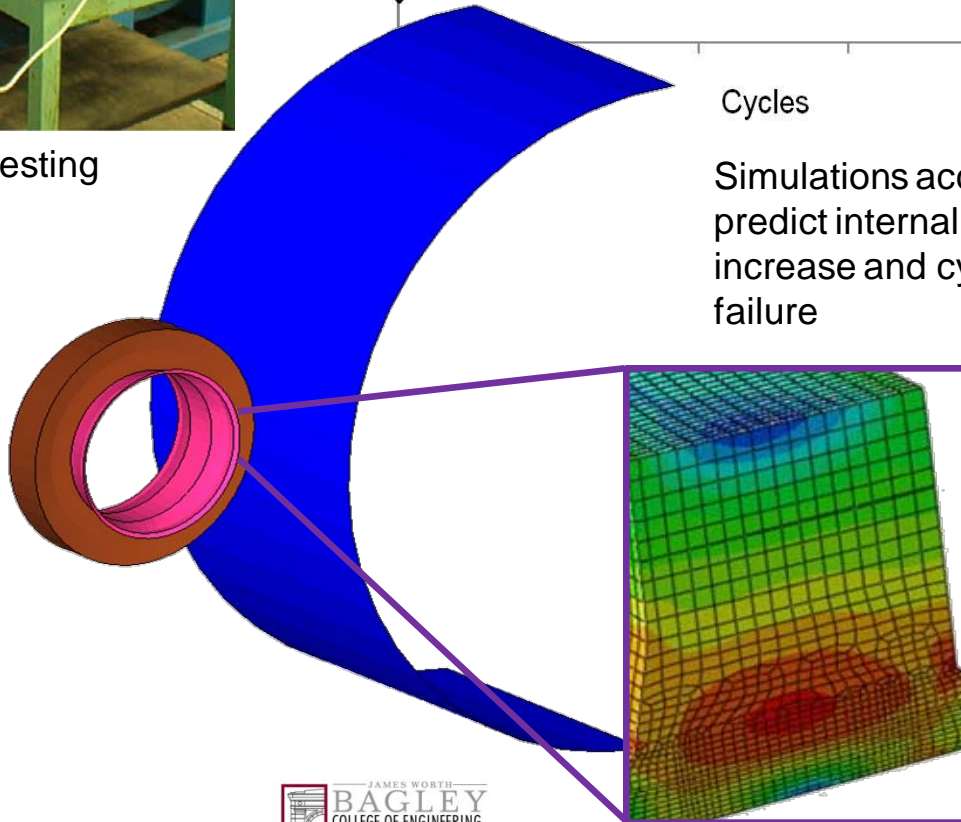
Component Life Prediction

Wheel dynamometer testing

Thermocouples embedded for internal measurements

Temperature

Cycles

Simulations accurately predict internal temperature increase and cycles to failure

Summary

1. Multidisciplinary Center

2. Lab equipment / Computational capability

3. Multiscale experiments

4. Multiscale modeling frameworks with ISV approach.

5. Application to Polyurethane insert component